Galerkin 3D

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1 Equations

1.1 Mass conservation

$$\frac{\partial c_i}{\partial t} = -\vec{\nabla}.\vec{N}_i + R_i \tag{1}$$

with

$$\vec{N}_i = c_i\vec{v} - \sum_j D_{ij}\vec{\nabla}c_j - w_i c_i \vec{\nabla}U \tag{2}$$

1.2 Poisson's equation

$$\vec{\nabla}^2 U + \frac{F}{\epsilon}\sum_i z_i c_i = 0 \tag{3}$$

1.3 Butler-Volmer kinetics

$$v = k_{ox}\exp\left[\frac{\alpha_{ox}nF}{RT}\left(V-U\right)\right]c_{red} - k_{red}\exp\left[-\frac{\alpha_{red}nF}{RT}\left(V-U\right)\right]c_{ox} \tag{4}$$

2 Element matrix

Note

$$\vec{\nabla}N^m = \frac{\vec{n}^m}{3V}$$

2.1 Convection

2.1.1 Fluctuation in node

$$\Delta c_i^m = \int_V -\vec{v}.\vec{\nabla}c_i N^m dV$$

2.1.2 Element contribution to fluctuation in node

Assume that $\vec{v}$ varies linearly.

$$\vec{\mathcal{V}}^1 = 2\vec{v}^1 + \vec{v}^2 + \vec{v}^3 + \vec{v}^4$$

$$\vec{\mathcal{V}}^2 = \vec{v}^1 + 2\vec{v}^2 + \vec{v}^3 + \vec{v}^4$$

$$\vec{\mathcal{V}}^3 = \vec{v}^1 + \vec{v}^2 + 2\vec{v}^3 + \vec{v}^4$$

$$\vec{\mathcal{V}}^4 = \vec{v}^1 + \vec{v}^2 + \vec{v}^3 + 2\vec{v}^4$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = \frac{1}{60} \left[\begin{array}{cccc} \vec{\mathcal{V}}^1.\vec{n}^1 & \vec{\mathcal{V}}^1.\vec{n}^2 & \vec{\mathcal{V}}^1.\vec{n}^3 & \vec{\mathcal{V}}^1.\vec{n}^4 \\ \vec{\mathcal{V}}^2.\vec{n}^1 & \vec{\mathcal{V}}^2.\vec{n}^2 & \vec{\mathcal{V}}^2.\vec{n}^3 & \vec{\mathcal{V}}^2.\vec{n}^4 \\ \vec{\mathcal{V}}^3.\vec{n}^1 & \vec{\mathcal{V}}^3.\vec{n}^2 & \vec{\mathcal{V}}^3.\vec{n}^3 & \vec{\mathcal{V}}^3.\vec{n}^4 \\ \vec{\mathcal{V}}^4.\vec{n}^1 & \vec{\mathcal{V}}^4.\vec{n}^2 & \vec{\mathcal{V}}^4.\vec{n}^3 & \vec{\mathcal{V}}^4.\vec{n}^4 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array} \right\} \tag{5}$$

2.1.3 Examples: binary electrolyte

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array} \right\} = \left[\begin{array}{cccccccccccc} V^{11} & 0 & 0 & V^{12} & 0 & 0 & V^{13} & 0 & 0 & V^{14} & 0 & 0 \\ 0 & V^{11} & 0 & 0 & V^{12} & 0 & 0 & V^{13} & 0 & 0 & V^{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V^{21} & 0 & 0 & V^{22} & 0 & 0 & V^{23} & 0 & 0 & V^{24} & 0 & 0 \\ 0 & V^{21} & 0 & 0 & V^{22} & 0 & 0 & V^{23} & 0 & 0 & V^{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V^{31} & 0 & 0 & V^{32} & 0 & 0 & V^{33} & 0 & 0 & V^{34} & 0 & 0 \\ 0 & V^{31} & 0 & 0 & V^{32} & 0 & 0 & V^{33} & 0 & 0 & V^{34} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V^{41} & 0 & 0 & V^{42} & 0 & 0 & V^{43} & 0 & 0 & V^{44} & 0 & 0 \\ 0 & V^{41} & 0 & 0 & V^{42} & 0 & 0 & V^{43} & 0 & 0 & V^{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array} \right\} \tag{6}$$

$$V^{mn} = \frac{\vec{\mathcal{V}}^m.\vec{n}^n}{60}$$

2.2 Diffusion

2.2.1 Fluctuation in node

$$\begin{aligned} \Delta c_i^m &= \int_V \vec{\nabla}.\left(\sum_j D_{ij}\vec{\nabla}c_j\right) N^m dV \\ &= -\int_V \left(\sum_j D_{ij}\vec{\nabla}c_j\right).\vec{\nabla}N^m dV \end{aligned}$$

2.2.2 Element contribution to fluctuation in node

Assume that D_{ij} varies linearly.

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = -\sum_j \frac{D_{ij}^1 + D_{ij}^2 + D_{ij}^3 + D_{ij}^4}{36V} \begin{bmatrix} \vec{n}^1.\vec{n}^1 & \vec{n}^1.\vec{n}^2 & \vec{n}^1.\vec{n}^3 & \vec{n}^1.\vec{n}^4 \\ \vec{n}^2.\vec{n}^1 & \vec{n}^2.\vec{n}^2 & \vec{n}^2.\vec{n}^3 & \vec{n}^2.\vec{n}^4 \\ \vec{n}^3.\vec{n}^1 & \vec{n}^3.\vec{n}^2 & \vec{n}^3.\vec{n}^3 & \vec{n}^3.\vec{n}^4 \\ \vec{n}^4.\vec{n}^1 & \vec{n}^4.\vec{n}^2 & \vec{n}^4.\vec{n}^3 & \vec{n}^4.\vec{n}^4 \end{bmatrix} \left\{ \begin{array}{c} c_j^1 \\ c_j^2 \\ c_j^3 \\ c_j^4 \end{array} \right\} \tag{7}$$

2.2.3 Example: binary electrolyte

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array} \right\} = \begin{bmatrix} D_{AA}^{11} & D_{AB}^{11} & 0 & D_{AA}^{12} & D_{AB}^{12} & 0 & D_{AA}^{13} & D_{AB}^{13} & 0 & D_{AA}^{14} & D_{AB}^{14} & 0 \\ D_{BA}^{11} & D_{BB}^{11} & 0 & D_{BA}^{12} & D_{BB}^{12} & 0 & D_{BA}^{13} & D_{BB}^{13} & 0 & D_{BA}^{14} & D_{BB}^{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ D_{AA}^{21} & D_{AB}^{21} & 0 & D_{AA}^{22} & D_{AB}^{22} & 0 & D_{AA}^{23} & D_{AB}^{23} & 0 & D_{AA}^{24} & D_{AB}^{24} & 0 \\ D_{BA}^{21} & D_{BB}^{21} & 0 & D_{BA}^{22} & D_{BB}^{22} & 0 & D_{BA}^{23} & D_{BB}^{23} & 0 & D_{BA}^{24} & D_{BB}^{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ D_{AA}^{31} & D_{AB}^{31} & 0 & D_{AA}^{32} & D_{AB}^{32} & 0 & D_{AA}^{33} & D_{AB}^{33} & 0 & D_{AA}^{34} & D_{AB}^{34} & 0 \\ D_{BA}^{31} & D_{BB}^{31} & 0 & D_{BA}^{32} & D_{BB}^{32} & 0 & D_{BA}^{33} & D_{BB}^{33} & 0 & D_{BA}^{34} & D_{BB}^{34} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ D_{AA}^{41} & D_{AB}^{41} & 0 & D_{AA}^{42} & D_{AB}^{42} & 0 & D_{AA}^{43} & D_{AB}^{43} & 0 & D_{AA}^{44} & D_{AB}^{44} & 0 \\ D_{BA}^{41} & D_{BB}^{41} & 0 & D_{BA}^{42} & D_{BB}^{42} & 0 & D_{BA}^{43} & D_{BB}^{43} & 0 & D_{BA}^{44} & D_{BB}^{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \left\{ \begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array} \right\} \tag{8}$$

with

$$D_{ij}^{mn} = -\frac{D_{ij}^1 + D_{ij}^2 + D_{ij}^3 + D_{ij}^4}{36V} \vec{n}^m.\vec{n}^n$$

2.3 Migration

2.3.1 Fluctuation in node

$$\begin{aligned} \Delta c_i^m &= \int_V \vec{\nabla}.\left(w_i c_i \vec{\nabla} U\right) N^m dV \\ &= -\int_V \left(w_i c_i \vec{\nabla} U\right).\vec{\nabla} N^m dV \end{aligned}$$

2.3.2 Element contribution to fluctuation in node

Assume that w_i varies linearly.

$$\mathcal{W}_i^1 = 2w_i^1 + w_i^2 + w_i^3 + w_i^4$$

$$\mathcal{W}_i^2 = w_i^1 + 2w_i^2 + w_i^3 + w_i^4$$

$$\mathcal{W}_i^3 = w_i^1 + w_i^2 + 2w_i^3 + w_i^4$$

$$\mathcal{W}_i^4 = w_i^1 + w_i^2 + w_i^3 + 2w_i^4$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = -\frac{\mathcal{W}_i^1 c_i^1 + \mathcal{W}_i^2 c_i^2 + \mathcal{W}_i^3 c_i^3 + \mathcal{W}_i^4 c_i^4}{180V} \left[\begin{array}{cccc} \vec{n}^1.\vec{n}^1 & \vec{n}^1.\vec{n}^2 & \vec{n}^1.\vec{n}^3 & \vec{n}^1.\vec{n}^4 \\ \vec{n}^2.\vec{n}^1 & \vec{n}^2.\vec{n}^2 & \vec{n}^2.\vec{n}^3 & \vec{n}^2.\vec{n}^4 \\ \vec{n}^3.\vec{n}^1 & \vec{n}^3.\vec{n}^2 & \vec{n}^3.\vec{n}^3 & \vec{n}^3.\vec{n}^4 \\ \vec{n}^4.\vec{n}^1 & \vec{n}^4.\vec{n}^2 & \vec{n}^4.\vec{n}^3 & \vec{n}^4.\vec{n}^4 \end{array} \right] \left\{ \begin{array}{c} U^1 \\ U^2 \\ U^3 \\ U^4 \end{array} \right\} \tag{9}$$

2.3.3 Example: binary electrolyte

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array} \right\} = \left[\begin{array}{cccccccccccc} 0 & 0 & M_A^{11} & 0 & 0 & M_A^{12} & 0 & 0 & M_A^{13} & 0 & 0 & M_A^{14} \\ 0 & 0 & M_B^{11} & 0 & 0 & M_B^{12} & 0 & 0 & M_B^{13} & 0 & 0 & M_B^{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & M_A^{21} & 0 & 0 & M_A^{22} & 0 & 0 & M_A^{23} & 0 & 0 & M_A^{24} \\ 0 & 0 & M_B^{21} & 0 & 0 & M_B^{22} & 0 & 0 & M_B^{23} & 0 & 0 & M_B^{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & M_A^{31} & 0 & 0 & M_A^{32} & 0 & 0 & M_A^{33} & 0 & 0 & M_A^{34} \\ 0 & 0 & M_B^{31} & 0 & 0 & M_B^{32} & 0 & 0 & M_B^{33} & 0 & 0 & M_B^{34} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & M_A^{41} & 0 & 0 & M_A^{42} & 0 & 0 & M_A^{43} & 0 & 0 & M_A^{44} \\ 0 & 0 & M_B^{41} & 0 & 0 & M_B^{42} & 0 & 0 & M_B^{43} & 0 & 0 & M_B^{44} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array} \right\} \tag{10}$$

with

$$M_i^{mn} = -\frac{\mathcal{W}_i^1 c_i^1 + \mathcal{W}_i^2 c_i^2 + \mathcal{W}_i^3 c_i^3 + \mathcal{W}_i^4 c_i^4}{180V} \vec{n}^m.\vec{n}^n$$

2.4 Homogeneous reactions

2.4.1 Fluctuation in node

$$R_i = \sum_r s_{i,r} v_r$$

- Monomolecular

$$v = kc_j$$

$$\Delta c_i^m = \int_V kc_j N^m dV$$

- Bimolecular

$$v = kc_j c_k$$

$$\begin{array}{rcl} \Delta c_i^m & = & \int_V kc_j c_k N^m dV \\ & = & \frac{1}{2}\int_V kc_k c_j N^m dV + \frac{1}{2}\int_V kc_j c_k N^m dV \end{array}$$

2.4.2 Element contribution to fluctuation in node

Assume that k varies linearly.

- Monomolecular

$$\mathcal{H}_j^{11} = 6k^1 + 2k^2 + 2k^3 + 2k^4$$

$$\mathcal{H}_j^{22} = 2k^1 + 6k^2 + 2k^3 + 2k^4$$

$$\mathcal{H}_j^{33} = 2k^1 + 2k^2 + 6k^3 + 2k^4$$

$$\mathcal{H}_j^{44} = 2k^1 + 2k^2 + 2k^3 + 6k^4$$

$$\mathcal{H}_j^{12} = \mathcal{H}_j^{21} = 2k^1 + 2k^2 + k^3 + k^4$$

$$\mathcal{H}_j^{13} = \mathcal{H}_j^{31} = 2k^1 + k^2 + 2k^3 + k^4$$

$$\mathcal{H}_j^{14} = \mathcal{H}_j^{41} = 2k^1 + k^2 + k^3 + 2k^4$$

$$\mathcal{H}_j^{23} = \mathcal{H}_j^{32} = k^1 + 2k^2 + 2k^3 + k^4$$

$$\mathcal{H}_j^{24} = \mathcal{H}_j^{42} = k^1 + 2k^2 + k^3 + 2k^4$$

$$\mathcal{H}_j^{34} = \mathcal{H}_j^{43} = k^1 + k^2 + 2k^3 + 2k^4$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = \frac{V}{120} \begin{bmatrix} \mathcal{H}_j^{11} & \mathcal{H}_j^{12} & \mathcal{H}_j^{13} & \mathcal{H}_j^{14} \\ \mathcal{H}_j^{21} & \mathcal{H}_j^{22} & \mathcal{H}_j^{23} & \mathcal{H}_j^{24} \\ \mathcal{H}_j^{31} & \mathcal{H}_j^{32} & \mathcal{H}_j^{33} & \mathcal{H}_j^{34} \\ \mathcal{H}_j^{41} & \mathcal{H}_j^{42} & \mathcal{H}_j^{43} & \mathcal{H}_j^{44} \end{bmatrix} \left\{ \begin{array}{c} c_j^1 \\ c_j^2 \\ c_j^3 \\ c_j^4 \end{array} \right\} \tag{11}$$

- Bimolecular

$$\mathcal{K}^{111} = 12k^1 + 3k^2 + 3k^3 + 3k^4$$

$$\mathcal{K}^{222} = 3k^1 + 12k^2 + 3k^3 + 3k^4$$

$$\mathcal{K}^{333} = 3k^1 + 3k^2 + 12k^3 + 3k^4$$

$$\mathcal{K}^{444} = 3k^1 + 3k^2 + 3k^3 + 12k^4$$

$$\mathcal{K}^{112} = \mathcal{K}^{121} = \mathcal{K}^{211} = 3k^1 + 2k^2 + k^3 + k^4$$

$$\mathcal{K}^{113} = \mathcal{K}^{131} = \mathcal{K}^{311} = 3k^1 + k^2 + 2k^3 + 1k^4$$

$$\mathcal{K}^{114} = \mathcal{K}^{141} = \mathcal{K}^{411} = 3k^1 + k^2 + k^3 + 2k^4$$

$$\mathcal{K}^{221} = \mathcal{K}^{122} = \mathcal{K}^{212} = 2k^1 + 3k^2 + k^3 + k^4$$

$$\mathcal{K}^{223} = \mathcal{K}^{232} = \mathcal{K}^{322} = k^1 + 3k^2 + 2k^3 + k^4$$

$$\mathcal{K}^{224} = \mathcal{K}^{242} = \mathcal{K}^{422} = k^1 + 3k^2 + k^3 + 2k^4$$

$$\mathcal{K}^{331} = \mathcal{K}^{133} = \mathcal{K}^{313} = 2k^1 + k^2 + 3k^3 + k^4$$

$$\mathcal{K}^{332} = \mathcal{K}^{233} = \mathcal{K}^{323} = k^1 + 2k^2 + 3k^3 + k^4$$

$$\mathcal{K}^{334} = \mathcal{K}^{343} = \mathcal{K}^{433} = k^1 + k^2 + 3k^3 + 2k^4$$

$$\mathcal{K}^{441} = \mathcal{K}^{144} = \mathcal{K}^{414} = 2k^1 + k^2 + k^3 + 3k^4$$

$$\mathcal{K}^{442} = \mathcal{K}^{244} = \mathcal{K}^{424} = k^1 + 2k^2 + k^3 + 3k^4$$

$$\mathcal{K}^{443} = \mathcal{K}^{344} = \mathcal{K}^{434} = k^1 + k^2 + 2k^3 + 3k^4$$

$$\mathcal{K}^{123} = \mathcal{K}^{213} = \mathcal{K}^{132} = \mathcal{K}^{312} = \mathcal{K}^{231} = \mathcal{K}^{321} = k^1 + k^2 + k^3 + \frac{k^4}{2}$$

$$\mathcal{K}^{124} = \mathcal{K}^{214} = \mathcal{K}^{142} = \mathcal{K}^{412} = \mathcal{K}^{241} = \mathcal{K}^{421} = k^1 + k^2 + \frac{k^3}{2} + k^4$$

$$\mathcal{K}^{134} = \mathcal{K}^{314} = \mathcal{K}^{143} = \mathcal{K}^{413} = \mathcal{K}^{341} = \mathcal{K}^{431} = k^1 + \frac{k^2}{2} + k^3 + k^4$$

$$\mathcal{K}^{234} = \mathcal{K}^{324} = \mathcal{K}^{243} = \mathcal{K}^{423} = \mathcal{K}^{342} = \mathcal{K}^{432} = \frac{k^1}{2} + k^2 + k^3 + k^4$$

$$\mathcal{H}_j^{11} = \mathcal{K}^{111} c_k^1 + \mathcal{K}^{112} c_k^2 + \mathcal{K}^{113} c_k^3 + \mathcal{K}^{114} c_k^4$$

$$\mathcal{H}_j^{22} = \mathcal{K}^{221} c_k^1 + \mathcal{K}^{222} c_k^2 + \mathcal{K}^{223} c_k^3 + \mathcal{K}^{224} c_k^4$$

$$\mathcal{H}_j^{33} = \mathcal{K}^{331} c_k^1 + \mathcal{K}^{332} c_k^2 + \mathcal{K}^{333} c_k^3 + \mathcal{K}^{334} c_k^4$$

$$\mathcal{H}_j^{44} = \mathcal{K}^{441} c_k^1 + \mathcal{K}^{442} c_k^2 + \mathcal{K}^{443} c_k^3 + \mathcal{K}^{444} c_k^4$$

$$\mathcal{H}_j^{12} = \mathcal{H}_j^{21} = \mathcal{K}^{121} c_k^1 + \mathcal{K}^{122} c_k^2 + \mathcal{K}^{123} c_k^3 + \mathcal{K}^{124} c_k^4$$

$$\mathcal{H}_j^{13} = \mathcal{H}_j^{31} = \mathcal{K}^{131} c_k^1 + \mathcal{K}^{132} c_k^2 + \mathcal{K}^{133} c_k^3 + \mathcal{K}^{134} c_k^4$$

$$\mathcal{H}_j^{14} = \mathcal{H}_j^{41} = \mathcal{K}^{141} c_k^1 + \mathcal{K}^{142} c_k^2 + \mathcal{K}^{143} c_k^3 + \mathcal{K}^{144} c_k^4$$

$$\mathcal{H}_j^{23} = \mathcal{H}_j^{32} = \mathcal{K}^{231} c_k^1 + \mathcal{K}^{232} c_k^2 + \mathcal{K}^{233} c_k^3 + \mathcal{K}^{234} c_k^4$$

$$\mathcal{H}_j^{24} = \mathcal{H}_j^{42} = \mathcal{K}^{241} c_k^1 + \mathcal{K}^{242} c_k^2 + \mathcal{K}^{243} c_k^3 + \mathcal{K}^{244} c_k^4$$

$$\mathcal{H}_j^{34} = \mathcal{H}_j^{43} = \mathcal{K}^{341} c_k^1 + \mathcal{K}^{342} c_k^2 + \mathcal{K}^{343} c_k^3 + \mathcal{K}^{344} c_k^4$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = \frac{V}{840} \left[\begin{array}{cccccccc} \mathcal{H}_j^{11} & \mathcal{H}_k^{11} & \mathcal{H}_j^{12} & \mathcal{H}_k^{12} & \mathcal{H}_j^{13} & \mathcal{H}_k^{13} & \mathcal{H}_j^{14} & \mathcal{H}_k^{14} \\ \mathcal{H}_j^{21} & \mathcal{H}_k^{21} & \mathcal{H}_j^{22} & \mathcal{H}_k^{22} & \mathcal{H}_j^{23} & \mathcal{H}_k^{23} & \mathcal{H}_j^{24} & \mathcal{H}_k^{24} \\ \mathcal{H}_j^{31} & \mathcal{H}_k^{31} & \mathcal{H}_j^{32} & \mathcal{H}_k^{32} & \mathcal{H}_j^{33} & \mathcal{H}_k^{33} & \mathcal{H}_j^{34} & \mathcal{H}_k^{34} \\ \mathcal{H}_j^{41} & \mathcal{H}_k^{41} & \mathcal{H}_j^{42} & \mathcal{H}_k^{42} & \mathcal{H}_j^{43} & \mathcal{H}_k^{43} & \mathcal{H}_j^{44} & \mathcal{H}_k^{44} \end{array} \right] \left\{ \begin{array}{c} c_j^1 \\ c_k^1 \\ c_j^2 \\ c_k^2 \\ c_j^3 \\ c_k^3 \\ c_j^4 \\ c_k^4 \end{array} \right\} \tag{12}$$

2.4.3 Example: monomolecular-monomolecular reversible reaction $A \rightleftharpoons B$

$$v = k_f c_A - k_b c_B$$

$$R_A = -v$$

$$R_B = v$$

$$\left\{\begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array}\right\} = \left[\begin{array}{cccccccccccc} -H_A^{11} & H_B^{11} & 0 & -H_A^{12} & H_B^{12} & 0 & -H_A^{13} & H_B^{13} & 0 & -H_A^{14} & H_B^{14} & 0 \\ H_A^{11} & -H_B^{11} & 0 & H_A^{12} & -H_B^{12} & 0 & H_A^{13} & -H_B^{13} & 0 & H_A^{14} & -H_B^{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -H_A^{21} & H_B^{21} & 0 & -H_A^{22} & H_B^{22} & 0 & -H_A^{23} & H_B^{23} & 0 & -H_A^{24} & H_B^{24} & 0 \\ H_A^{21} & -H_B^{21} & 0 & H_A^{22} & -H_B^{22} & 0 & H_A^{23} & -H_B^{23} & 0 & H_A^{24} & -H_B^{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -H_A^{31} & H_B^{31} & 0 & -H_A^{32} & H_B^{32} & 0 & -H_A^{33} & H_B^{33} & 0 & -H_A^{34} & H_B^{34} & 0 \\ H_A^{31} & -H_B^{31} & 0 & H_A^{32} & -H_B^{32} & 0 & H_A^{33} & -H_B^{33} & 0 & H_A^{34} & -H_B^{34} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -H_A^{41} & H_B^{41} & 0 & -H_A^{42} & H_B^{42} & 0 & -H_A^{43} & H_B^{43} & 0 & -H_A^{44} & H_B^{44} & 0 \\ H_A^{41} & -H_B^{41} & 0 & H_A^{42} & -H_B^{42} & 0 & H_A^{43} & -H_B^{43} & 0 & H_A^{44} & -H_B^{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \left\{\begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array}\right\} \tag{13}$$

with for the forward reaction (replace k by k_f in the formulae!)

$$H_A^{mn} = \frac{V}{120}\mathcal{H}_A^{mn}$$

and for the backward reaction (replace k by k_b in the formulae!)

$$H_B^{mn} = \frac{V}{120}\mathcal{H}_B^{mn}$$

2.5 Poisson's equation

2.5.1 Fluctuation in node

$$\begin{array}{rcl} \Delta U^m & = & \int_V \vec{\nabla}^2 U N^m dV + \int_V \frac{F}{\epsilon} \sum_i z_i c_i N^m dV \\ & = & -\int_V \vec{\nabla} U . \vec{\nabla} N^m dV + \sum_i \frac{z_i F}{\epsilon} \int_V c_i N^m dV \end{array}$$

2.5.2 Element contribution to fluctuation in node

$$\left\{\begin{array}{c} \Delta U^1 \\ \Delta U^2 \\ \Delta U^3 \\ \Delta U^4 \end{array}\right\} = \left[\begin{array}{cccccccc} \frac{2V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^1.\vec{n}^1}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^1.\vec{n}^2}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^1.\vec{n}^3}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^1.\vec{n}^4}{9V} \\ \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^2.\vec{n}^1}{9V} & \frac{2V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^2.\vec{n}^2}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^2.\vec{n}^3}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^2.\vec{n}^4}{9V} \\ \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^3.\vec{n}^1}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^3.\vec{n}^2}{9V} & \frac{2V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^3.\vec{n}^3}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^3.\vec{n}^4}{9V} \\ \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^4.\vec{n}^1}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^4.\vec{n}^2}{9V} & \frac{V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^4.\vec{n}^3}{9V} & \frac{2V}{20}\frac{z_iF}{\epsilon} & -\frac{\vec{n}^4.\vec{n}^4}{9V} \end{array}\right] \left\{\begin{array}{c} c_i^1 \\ U^1 \\ c_i^2 \\ U^2 \\ c_i^3 \\ U^3 \\ c_i^4 \\ U^4 \end{array}\right\} \tag{14}$$

2.5.3 Example: binary electrolyte

$$\left\{\begin{matrix} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{matrix}\right\} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2Z_A & 2Z_B & n^{11} & Z_A & Z_B & n^{12} & Z_A & Z_B & n^{13} & Z_A & Z_B & n^{14} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ Z_A & Z_B & n^{21} & 2Z_A & 2Z_B & n^{22} & Z_A & Z_B & n^{23} & Z_A & Z_B & n^{24} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ Z_A & Z_B & n^{31} & Z_A & Z_B & n^{32} & 2Z_A & 2Z_B & n^{33} & Z_A & Z_B & n^{34} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ Z_A & Z_B & n^{41} & Z_A & Z_B & n^{42} & Z_A & Z_B & n^{43} & 2Z_A & 2Z_B & n^{44} \end{bmatrix} \left\{\begin{matrix} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{matrix}\right\} \tag{15}$$

with

$$Z_i = \frac{V}{20}\frac{z_i F}{\epsilon}$$

$$n^{mn} = -\frac{\vec{n}^m . \vec{n}^n}{9V}$$

2.6 Time

2.6.1 Fluctuation in node

$$\Delta c_i^m = \int_V \frac{\partial c_i}{\partial t} N^m dV$$

2.6.2 Element contribution to fluctuation in node

$$\left\{\begin{matrix} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{matrix}\right\} = \frac{V}{20}\begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \left\{\begin{matrix} \frac{\partial c_i^1}{\partial t} \\ \frac{\partial c_i^2}{\partial t} \\ \frac{\partial c_i^3}{\partial t} \\ \frac{\partial c_i^4}{\partial t} \end{matrix}\right\} \tag{16}$$

3 Boundary element vector

3.1 Electrode reactions

3.1.1 Fluctuation in node

$$R_i = \sum_r s_{i,r} v_r$$

$$v = k_{ox} \exp\left[\frac{\alpha_{ox} n F}{RT}(V-U)\right] c_{red} - k_{red} \exp\left[-\frac{\alpha_{red} n F}{RT}(V-U)\right] c_{ox}$$

$$\Delta c_i^m = \int_S R_i N^m dS$$

3.1.2 Boundary element contribution to fluctuation in node

Assume that the normal flux varies linearly on the boundary.

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \end{array} \right\} = \frac{S}{12} \left\{ \begin{array}{c} 2R_i^1 + R_i^2 + R_i^3 \\ R_i^1 + 2R_i^2 + R_i^3 \\ R_i^1 + R_i^2 + 2R_i^3 \end{array} \right\} \tag{17}$$

3.1.3 Example: binary electrolyte, $A \rightleftharpoons B + ne^-$

$$v = k_{ox} \exp\left[\frac{\alpha_{ox} nF}{RT}(V-U)\right] c_B - k_{red} \exp\left[-\frac{\alpha_{red} nF}{RT}(V-U)\right] c_A$$

$$R_A = -v$$

$$R_B = v$$

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \end{array} \right\} = \left\{ \begin{array}{c} -\frac{S}{12}\left(2v^1 + v^2 + v^3\right) \\ \frac{S}{12}\left(2v^1 + v^2 + v^3\right) \\ 0 \\ -\frac{S}{12}\left(v^1 + 2v^2 + v^3\right) \\ \frac{S}{12}\left(v^1 + 2v^2 + v^3\right) \\ 0 \\ -\frac{S}{12}\left(v^1 + v^2 + 2v^3\right) \\ \frac{S}{12}\left(v^1 + v^2 + 2v^3\right) \\ 0 \end{array} \right\} \tag{18}$$

4 Element jacobian

4.1 Convection

Zero contribution.

4.2 Diffusion

Zero contribution (approximately).

4.3 Migration

4.3.1 Element contribution to fluctuation in node

$$\vec{\nabla} U = \frac{\vec{n}^1 U^1 + \vec{n}^2 U^2 + \vec{n}^3 U^3 + \vec{n}^4 U^4}{3V}$$

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = -\frac{\vec{\nabla} U}{60} . \left[\begin{array}{cccc} \vec{n}^1 \mathcal{W}_i^1 & \vec{n}^1 \mathcal{W}_i^2 & \vec{n}^1 \mathcal{W}_i^3 & \vec{n}^1 \mathcal{W}_i^4 \\ \vec{n}^2 \mathcal{W}_i^1 & \vec{n}^2 \mathcal{W}_i^2 & \vec{n}^2 \mathcal{W}_i^3 & \vec{n}^2 \mathcal{W}_i^4 \\ \vec{n}^3 \mathcal{W}_i^1 & \vec{n}^3 \mathcal{W}_i^2 & \vec{n}^3 \mathcal{W}_i^3 & \vec{n}^3 \mathcal{W}_i^4 \\ \vec{n}^4 \mathcal{W}_i^1 & \vec{n}^4 \mathcal{W}_i^2 & \vec{n}^4 \mathcal{W}_i^3 & \vec{n}^4 \mathcal{W}_i^4 \end{array} \right] \left\{ \begin{array}{c} c_i^1 \\ c_i^2 \\ c_i^3 \\ c_i^4 \end{array} \right\} \tag{19}$$

4.3.2 Example: binary electrolyte

$$\left\{ \begin{array}{c} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \\ \Delta c_A^4 \\ \Delta c_B^4 \\ \Delta U^4 \end{array} \right\} = \left[\begin{array}{cccccccccccc} \tilde{M}_A^{11} & 0 & 0 & \tilde{M}_A^{12} & 0 & 0 & \tilde{M}_A^{13} & 0 & 0 & \tilde{M}_A^{14} & 0 & 0 \\ 0 & \tilde{M}_B^{11} & 0 & 0 & \tilde{M}_B^{12} & 0 & 0 & \tilde{M}_B^{13} & 0 & 0 & \tilde{M}_B^{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \tilde{M}_A^{21} & 0 & 0 & \tilde{M}_A^{22} & 0 & 0 & \tilde{M}_A^{23} & 0 & 0 & \tilde{M}_A^{24} & 0 & 0 \\ 0 & \tilde{M}_B^{21} & 0 & 0 & \tilde{M}_B^{22} & 0 & 0 & \tilde{M}_B^{23} & 0 & 0 & \tilde{M}_B^{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \tilde{M}_A^{31} & 0 & 0 & \tilde{M}_A^{32} & 0 & 0 & \tilde{M}_A^{33} & 0 & 0 & \tilde{M}_A^{34} & 0 & 0 \\ 0 & \tilde{M}_B^{31} & 0 & 0 & \tilde{M}_B^{32} & 0 & 0 & \tilde{M}_B^{33} & 0 & 0 & \tilde{M}_B^{34} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \tilde{M}_A^{41} & 0 & 0 & \tilde{M}_A^{42} & 0 & 0 & \tilde{M}_A^{43} & 0 & 0 & \tilde{M}_A^{44} & 0 & 0 \\ 0 & \tilde{M}_B^{41} & 0 & 0 & \tilde{M}_B^{42} & 0 & 0 & \tilde{M}_B^{43} & 0 & 0 & \tilde{M}_B^{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \left\{ \begin{array}{c} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \\ c_A^4 \\ c_B^4 \\ U^4 \end{array} \right\} \tag{20}$$

with

$$\tilde{M}_i^{mn} = -\vec{\nabla} U . \vec{n}^m \frac{\mathcal{W}_i^n}{60}$$

4.4 Homogeneous reactions

4.4.1 Element contribution to fluctuation in node

- Monomolecular

Zero contribution (approximately).

- Bimolecular

Because of the symmetry it is the same contribution.

$$\left\{ \begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \\ \Delta c_i^4 \end{array} \right\} = \frac{V}{840} \left[\begin{array}{cccccccc} \mathcal{H}_j^{11} & \mathcal{H}_k^{11} & \mathcal{H}_j^{12} & \mathcal{H}_k^{12} & \mathcal{H}_j^{13} & \mathcal{H}_k^{13} & \mathcal{H}_j^{14} & \mathcal{H}_k^{14} \\ \mathcal{H}_j^{21} & \mathcal{H}_k^{21} & \mathcal{H}_j^{22} & \mathcal{H}_k^{22} & \mathcal{H}_j^{23} & \mathcal{H}_k^{23} & \mathcal{H}_j^{24} & \mathcal{H}_k^{24} \\ \mathcal{H}_j^{31} & \mathcal{H}_k^{31} & \mathcal{H}_j^{32} & \mathcal{H}_k^{32} & \mathcal{H}_j^{33} & \mathcal{H}_k^{33} & \mathcal{H}_j^{34} & \mathcal{H}_k^{34} \\ \mathcal{H}_j^{41} & \mathcal{H}_k^{41} & \mathcal{H}_j^{42} & \mathcal{H}_k^{42} & \mathcal{H}_j^{43} & \mathcal{H}_k^{43} & \mathcal{H}_j^{44} & \mathcal{H}_k^{44} \end{array} \right] \left\{ \begin{array}{c} c_j^1 \\ c_k^1 \\ c_j^2 \\ c_k^2 \\ c_j^3 \\ c_k^3 \\ c_j^4 \\ c_k^4 \end{array} \right\} \tag{21}$$

4.5 Poisson's equation

Zero contribution.

4.6 Time

Zero contribution.

5 Boundary element jacobian

5.1 Electrode reactions

5.1.1 Partial derivatives

$$\frac{\partial v}{\partial U} = -\frac{\alpha_{ox} nF}{RT} k_{ox} \exp\left[\frac{\alpha_{ox} nF}{RT}\left(V-U\right)\right] c_{red} - \frac{\alpha_{red} nF}{RT} k_{red} \exp\left[-\frac{\alpha_{red} nF}{RT}\left(V-U\right)\right] c_{ox}$$

$$\frac{\partial v}{\partial c_{ox}} = -k_{red} \exp\left[-\frac{\alpha_{red} nF}{RT}\left(V-U\right)\right]$$

$$\frac{\partial v}{\partial c_{red}} = k_{ox} \exp\left[\frac{\alpha_{ox} nF}{RT}\left(V-U\right)\right]$$

$$\left\{\begin{array}{c} \Delta c_i^1 \\ \Delta c_i^2 \\ \Delta c_i^3 \end{array}\right\} = \frac{S}{12}\left[\begin{array}{cccccc} 2\frac{\partial R_i^1}{\partial c_j^1} & 2\frac{\partial R_i^1}{\partial U^1} & \frac{\partial R_i^2}{\partial c_j^2} & \frac{\partial R_i^2}{\partial U^2} & \frac{\partial R_i^3}{\partial c_j^3} & \frac{\partial R_i^3}{\partial U^3} \\ \frac{\partial R_i^1}{\partial c_j^1} & \frac{\partial R_i^1}{\partial U^1} & 2\frac{\partial R_i^2}{\partial c_j^2} & 2\frac{\partial R_i^2}{\partial U^2} & \frac{\partial R}{\partial c_j^3} & \frac{\partial R_i^3}{\partial U^3} \\ \frac{\partial R_i^1}{\partial c_j^1} & \frac{\partial R_i^1}{\partial U^1} & \frac{\partial R_i^2}{\partial c_j^2} & \frac{\partial R_i^2}{\partial U^2} & 2\frac{\partial R_i^3}{\partial c_j^3} & 2\frac{\partial R_i^3}{\partial U^3} \end{array}\right]\left\{\begin{array}{c} c_j^1 \\ U^1 \\ c_j^2 \\ U^2 \\ c_j^3 \\ U^3 \end{array}\right\} \tag{22}$$

5.1.2 Example: binary electrolyte, $A \rightleftharpoons B + ne^-$

$$\frac{\partial v}{\partial U} = -\frac{\alpha_{ox} nF}{RT} k_{ox} \exp\left[\frac{\alpha_{ox} nF}{RT}\left(V-U\right)\right] c_B - \frac{\alpha_{red} nF}{RT} k_{red} \exp\left[-\frac{\alpha_{red} nF}{RT}\left(V-U\right)\right] c_A$$

$$\frac{\partial v}{\partial c_A} = -k_{red} \exp\left[-\frac{\alpha_{red} nF}{RT}\left(V-U\right)\right]$$

$$\frac{\partial v}{\partial c_B} = k_{ox} \exp\left[\frac{\alpha_{ox} nF}{RT}\left(V-U\right)\right]$$

$$
\begin{Bmatrix} \Delta c_A^1 \\ \Delta c_B^1 \\ \Delta U^1 \\ \Delta c_A^2 \\ \Delta c_B^2 \\ \Delta U^2 \\ \Delta c_A^3 \\ \Delta c_B^3 \\ \Delta U^3 \end{Bmatrix} = \begin{bmatrix} -2\tilde{C}_A^1 & -2\tilde{C}_B^1 & -2\tilde{U}^1 & -\tilde{C}_A^2 & -\tilde{C}_B^2 & -\tilde{U}^2 & -\tilde{C}_A^3 & -\tilde{C}_B^3 & -\tilde{U}^3 \\ 2\tilde{C}_A^1 & 2\tilde{C}_B^1 & 2\tilde{U}^1 & \tilde{C}_A^2 & \tilde{C}_B^2 & \tilde{U}^2 & \tilde{C}_A^3 & \tilde{C}_B^3 & \tilde{U}^3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\tilde{C}_A^1 & -\tilde{C}_B^1 & -\tilde{U}^1 & -2\tilde{C}_A^2 & -2\tilde{C}_B^2 & -2\tilde{U}^2 & -\tilde{C}_A^3 & -\tilde{C}_B^3 & -\tilde{U}^3 \\ \tilde{C}_A^1 & \tilde{C}_B^1 & \tilde{U}^1 & 2\tilde{C}_A^2 & 2\tilde{C}_B^2 & 2\tilde{U}^2 & \tilde{C}_A^3 & \tilde{C}_B^3 & \tilde{U}^3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\tilde{C}_A^1 & -\tilde{C}_B^1 & -\tilde{U}^1 & -\tilde{C}_A^2 & -\tilde{C}_B^2 & -\tilde{U}^2 & -2\tilde{C}_A^3 & -2\tilde{C}_B^3 & -2\tilde{U}^3 \\ \tilde{C}_A^1 & \tilde{C}_B^1 & \tilde{U}^1 & \tilde{C}_A^2 & \tilde{C}_B^2 & \tilde{U}^2 & 2\tilde{C}_A^3 & 2\tilde{C}_B^3 & 2\tilde{U}^3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} c_A^1 \\ c_B^1 \\ U^1 \\ c_A^2 \\ c_B^2 \\ U^2 \\ c_A^3 \\ c_B^3 \\ U^3 \end{Bmatrix} \tag{23}
$$

with

$$
\tilde{C}_i^m = \frac{S}{12}\frac{\partial v^m}{\partial c_i^m}
$$

$$
\tilde{U}^m = \frac{S}{12}\frac{\partial v^m}{\partial U^m}
$$